Andreev Bound States in the Kondo Quantum Dots Coupled to Superconducting Leads

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We have studied the Kondo quantum dot coupled to two superconducting leads and investigated the subgap Andreev states using the NRG method. Contrary to the recent NCA results [Clerk and Ambegaokar, Phys. Rev. B 61, 9109 (2000); Sellier et al., Phys. Rev. B 72, 174502 (2005)], we observe Andreev states both below and above the Fermi level.

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When a localized spin (in an impurity or a quantum dot) coupled to BCS-type s-wave superconductors(S), two strong correlation effects compete. The superconductivity tends to keep the conduction electrons in singlet pairs[1], leaving the local spin unscreened. The spin state of the total wave function is thus a doublet. The Kondo effect tends to screen the local spin with the spins of the quasiparticle excitations in the superconductor. The total spin state is thus a singlet[2]. This competition gives rise to a quantum phase transition from the doublet to singlet state, and the transport properties are dramatically changed across this transition[3, 4]. For example, the Josephson current through the quantum dot (QD) coupled to two superconducting leads has a π-shift in its current-phase relation (a so-called π-junction behavior) for the doublet state, while it has a 0-junction behavior for the singlet state[5, 6, 7, 8, 9, 10, 11, 12, 13]. In fact, all the previous studies[5, 6, 7, 8, 9, 10, 11, 12, 13] of the transition between the doublet and singlet state focused on the current-phase relation $I_S(\phi)$ of the Josephson current.

However, there are another non-trivial issues, about the Andreev bound states in such a system. The issues are: (1) How many subgap Andreev states are there? (2) Are the subgap Andreev states true bound states or quasi-bound states with finite level broadening?

Using the non-crossing approximation (NCA), Clerk and Ambegaokar [7] investigated the close relation between the 0-π transition in $I_S(\phi)$ and the Andreev states. They found that there is only one subgap Andreev state and that the Andreev state is located below (above) the Fermi energy E_F in the doublet (singlet) state. They provided an intuitively appealing interpretation that in the doublet state, the impurity level well below E_F is singly occupied and due to the strong on-site interaction energy U only hole-like excitations are allowed. In the singlet state, a small probability to find the impurity empty, electron-like excitations are allowed. This result was supported further by a more elaborated NCA method by Sellier et al. [13]. As stressed by Clerk and Ambegaokar [7], this observation casts a strong contrast with the non-interacting case, where bound states always occur in pairs (below and above E_F)[14, 15]. Moreover, the Andreev state has a finite broadening.

To the contrary, the Hartree-Fock theory (HFT) [16] predicts two Andreev states both below and above E_F in the Kondo regime. This was in agreement with the numerical renormalization group (NRG) calculations by [17], who studied the Andreev states as a function of the impurity level position. Slave-boson mean-field theory (SBMFT) [18] also predicts both electron-like (above E_F) and hole-like (below E_F) Andreev states. Further, they both predict infinitely sharp Andreev states. However, HFT and SBMFT are effectively non-interacting theory and may not provide a strong argument against the NCA result. In a previous work[8] we observed both Andreev states in the NRG result, but the model had the particle-hole symmetry.

In this work, we report a systematic study of the issues using the NRG method. We find both electron-like and hole-like Andreev states except in the deep inside the doublet phase (superconducting gap even bigger than the hybridization). We also provide a supporting interpretation based on the variational wave functions suggested by Rozhkov and Arovas [6].

The subgap Andreev bound states are important because they are directly related to the transport properties of the S/QD/S systems as in the recent experiment[19, 20, 21, 22]. Recent developments in mesoscopic transport experiments may allow direct measurement of these Andreev states through tunneling spectroscopy. So far, the NCA/SNCA and the NRG are the only methods which can treat rather systematically the many-body correlations of the Anderson-type impurity coupled to superconductors. The discrepancy between the two methods may motivate further theoretical efforts for better understanding of the many-body states of the system.

Summary of the Results We consider a QD (or magnetic impurity) coupled to two superconducting leads. The Hamiltonian $H = H_C + H_D + H_T$ consists of three parts: H_C describes two, left (L) and right (R), BCS-like s-wave superconductors with the superconducting

gap $\Delta_{L(R)}$ and band width D

$$H_C = \sum_{\ell=L,R} \left[\sum_{k\sigma} \xi_{\ell k} c^\dagger_{\ell k\sigma} c_{\ell k\sigma} - \left(\Delta_\ell c^\dagger_{\ell k\uparrow} c_{\ell k\downarrow} + h.c. \right) \right] \tag{1}$$

We assume identical superconductors, $\xi_{Lk} = \xi_{Rk} = \xi_k$ and $\Delta_L = \Delta_R^* = \Delta e^{+i\phi/2}$, where ϕ is the phase difference between the two superconductors. H_D describes an Anderson-type single level in the QD

$$H_D = \sum_\sigma \epsilon_d d^\dagger_\sigma d_\sigma + U n_\uparrow n_\downarrow \tag{2}$$

with $n_\sigma = d^\dagger_\sigma d_\sigma$. ϵ_d is the single-particle energy of the level and U is the on-site interaction. Here we consider particle-hole *asymmetric* case ($\epsilon_d \neq -U/2$). To compare our results directly with the NCA results, we will mostly take $U = \infty$ by preventing double occupancy. Finally H_T is responsible for the the tunneling of electrons between the superconductors and the QD

$$H_T = \sum_{\ell k\sigma} \left(V_{\ell k} c^\dagger_{\ell k\sigma} d_\sigma + h.c. \right) \tag{3}$$

For simplicity we will assume the symmetric junctions with tunneling elements insensitive to the energy, $V_{Lk} = V_{Rk} = V$. The broadening of the level is given by $\Gamma = \pi\rho_L(E_F)|V_L|^2 + \pi\rho_R(E_F)|V_R|^2 = 2\pi\rho(E_F)|V|^2$. For the calculation, we followed the standard NRG method[23, 24, 25, 26, 27] extended to superconducting leads[17, 28, 29].

There are two competing energy scales in the system. The superconductivity is naturally governed by the gap Δ. The Kondo effect is characterized by the Kondo temperature T_K, given by[8, 11, 30, 31]

$$T_K = \sqrt{\frac{\Gamma W_0}{2}} \exp\left[\frac{\pi\epsilon_d}{2\Gamma} \left(1 + \frac{\epsilon_d}{U} \right) \right] \tag{4}$$

where $W_0 \equiv \min\{D, U\}$. For $T_K \gg \Delta$, the ground state is expected to be a singlet and the Josephson current is governed by the Kondo physics. In the opposite limit $T_K \ll \Delta$, the ground state is a doublet and the transport can be understood perturbatively in the spirit of the Coulomb blockade (CB) effect[4, 32]. The transition happens at $T_K \sim \Delta$. See Fig. 3.

Figure 1 summarizes the results. Figure 1 (a) shows the positions, E_e and E_h, of the subgap Andreev states for $U = \infty$ and $\phi = 0$. We observe two Andreev states, below and above E_F are observed in a wide range of Δ/T_K (in particular on both sides of the transition point $\Delta_c/T_K \sim 1$). More important are Fig. 1 (b) and (c), the spectral weights A_e (A_h) of the electron-like (hole-like) Andreev states, defined by

$$G^R_{dd}(E) \approx \frac{A_p}{E - E_p + i0^+} \tag{5}$$

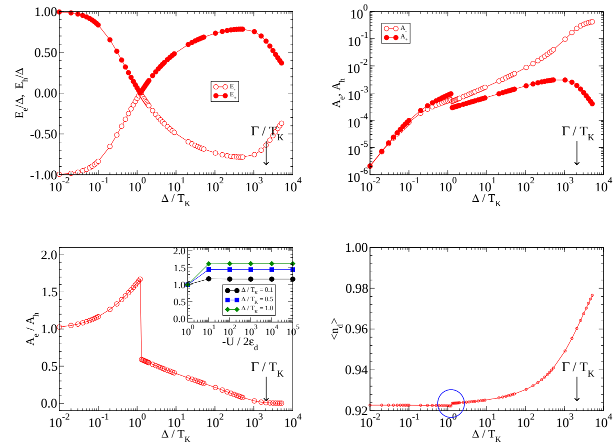

FIG. 1: (color on-line) The energies (a) and the corresponding spectral weights (b) of the subgap Andreev states for $U = \infty$ Anderson model. (c) The ratio A_e/A_h of the spectral weights of the Andreev states. Inset: A_e/A_h as a function of $-U/2\epsilon_d$. (d) Average occupation of the QD level. $\epsilon_d = -0.1D$, $U = \infty$, $\Gamma = 0.02D$ ($T_K \approx 3.88 \times 10^{-5}$).

near $E \simeq E_p$ ($p = e, h$). Except for very large Δ ($\Delta \gg \Gamma$), both E_e and E_h have order of magnitude the same spectral weights. These observations are consistent with the occupation of the dot level shown in Fig. 1 (d). Unlike the intuitive interpretation by [7], the occupation does not change much across the transition point, although there is a small jump [emphasized in the blue circle in Fig. 1 (d)]. The results in Fig. 1 remain qualitatively the same for finite U; an example is show in the inset of Fig. 1 (c). Finite phase difference (not shown in the figure) does not make any qualitative change (about the existance of the Andereev states both above and below E_F), either.

Variational Theory The main features of the results summarized above can be understood *qualitatively* in terms of the variational wave functions[6]. For the singlet state in the $U = \infty$ limit we take the trial function of the form

$$|S\rangle = \left\{ A + \frac{1}{\sqrt{2}} \sum_{q\in L,R} B_q (\gamma^\dagger_{q\uparrow} d^\dagger_\downarrow - \gamma^\dagger_{q\downarrow} d^\dagger_\uparrow) + \sum_{qq'} C_{qq'} \gamma^\dagger_{q\uparrow} \gamma^\dagger_{q'\downarrow} \right\} |0\rangle \tag{6}$$

with $C_{qq'} = C_{q'q}$. For the doublet state we take

$$|D_\uparrow\rangle = \left\{ \widetilde{A} d^\dagger_\uparrow + \sum_q \widetilde{B}_q \gamma^\dagger_{q\uparrow} + \sum_{qq'} \widetilde{C}_{qq'} \gamma^\dagger_{q\uparrow} \gamma^\dagger_{q'\downarrow} d^\dagger_\uparrow - \frac{1}{\sqrt{3}} \sum_{qq'} \widetilde{D}_{qq'} \gamma^\dagger_{q\uparrow} \left(\gamma^\dagger_{q'\uparrow} d_\downarrow - \gamma^\dagger_{q'\downarrow} d_\uparrow \right) \right\} |0\rangle \tag{7}$$

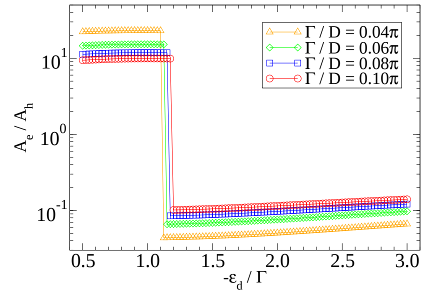

FIG. 2: (color on-line) Results from the variational calculations. Plotted is the Ratio A_e/A_h of the spectral weights as a function of $-\epsilon_d/\Gamma$ for various values of Γ. $\Delta/D = 0.1$.

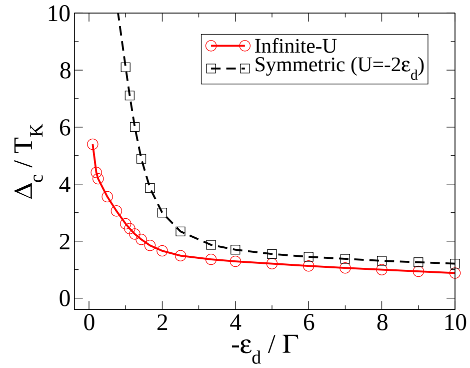

FIG. 3: (color on-line) Phase diagram of the Anderson impurity model with superconducting leads (for $\phi = 0$). The phase boundaries for the infinite-U model (red solid line with circles) and for the particle-hole symmetric model (black dashed line with squares), respectively, have been calculated by the NRG method.

with $\widetilde{C}_{qq'} = \widetilde{C}_{q'q}$ and $\widetilde{D}_{qq'} = -D_{q'q}$, and analogously $|D_\downarrow\rangle$. The coefficients in the trial wave functions are determined by minimizing $E = \langle\Psi|H\Psi\rangle/\langle\Psi|\Psi\rangle$ for $|\Psi\rangle = |S\rangle$ and $|\Psi\rangle = |D_\sigma\rangle$.

From the form of the trial wave functions, the spectral strength of the hole-like Andreev state in the singlet phase depends on how much the QD is occupied (B_q) in $|S\rangle$ and how much the QD is empty ($\widetilde{B}_q$) in $|D_\sigma\rangle$, namely, on the matrix element

$$\langle D_\uparrow|d_\downarrow|S\rangle = -\frac{1}{\sqrt{2}}\sum_q \widetilde{B}_q^*\widetilde{B}_q \tag{8}$$

(up to normalization constant $\sqrt{\langle S|S\rangle\langle D_\uparrow|D_\uparrow\rangle}$). The strength of the electron-like Andreev state in the doublet phase also depends on $\langle D_\uparrow|d_\downarrow|S\rangle$. Likewise, the strength of the electron-like (hole-like) Andreev state in the singlet (doublet) phase is determined by the matrix element

$$\langle D_\uparrow|d_\uparrow^\dagger|S\rangle = \widetilde{A}^* A + \sum_{qq'} \widetilde{C}_{qq'}^* C_{qq'}. \tag{9}$$

According to the NCA results[7, 13], $\langle D_\uparrow|d_\downarrow|S\rangle$ ($\langle D_\uparrow|d_\uparrow^\dagger|S\rangle$) should vanish in the singlet (doublet) phase. However, as shown in Fig. 2, neither of them vanishes, and the spectral weights A_e and A_h are similar in order of magnitude on both sides of the transition point, in agreement with the NRG results. We must point out that the agreement between the variational and NRG results is only at a qualitative level. The ratio A_e/A_h from the variational method is about 5 times bigger than the NRG result. However, this is not surprising because the variational method is limited in the regime T_K not too large compared with Δ; see below.

There is another interesting point to be noticed in the variational wave functions in Eqs. (6) and (7). The lowest-energy solution to the variational equation for $|S\rangle$ is well separated from the continuum. This is also true for $|D_\sigma\rangle$. This suggests that the subgap Andreev state

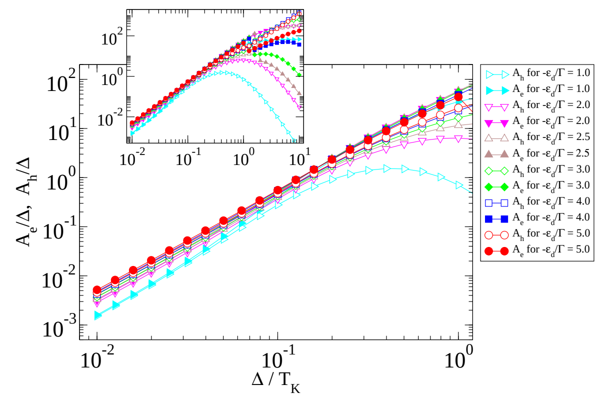

FIG. 4: (color on-line) Spectral weights A_e (A_h) of the electron-like (hole-like) Andreev state as a function of Δ/T_K at $\epsilon_d = \phi = 0$. Inset: the same in a wider range of Δ/T_K including the doublet phase.

is a true bound state without broadening. We will come back to this discussion below.

Universality Since the singlet-doublet transition in the system is a true quantum phase transition, the universality is also an important issue. With Δ and T_K being the only two low energy scales in the system, physical quantities should depend only on the ratio of Δ/T_K but not on the details of the system.

In Fig. 4, we plotted the normalized spectral weights $A_{e(h)}/\Delta$ as a function of Δ/T_K for various values of ϵ_d/Γ. We observe that the curves of $A_{e(h)}$ overlap each other almost completely in the Kondo regime ($\Delta \ll T_K$) except for cases close to the mixed-valence regime ($|\epsilon_d| \lesssim \Gamma$). The deviation from the universal behavior in the mixed-valence regime ($-\epsilon_d \lesssim \Gamma$) is not surprising because of strong charge fluctuations in the regime. This is also indicated the phase diagram in Fig. 3: Close to the mixed-valence regime ($-\epsilon_d/\Gamma \lesssim 1$), Δ_c/T_K becomes larger.

More interestingly, the universal curve in Fig. 4 can fit

to a simple effective non-interacting model. On a non-interacting resonance level coupled to two superconducting reservoirs, the spectral weights of the Andreev states are given by

$$\frac{A_{e(h)}}{\Delta} = \frac{(1-\omega_0^2)}{\mathcal{D}'(\omega_0)\mathcal{D}(\omega_0)}\left[z\left(1+\frac{\Gamma}{\sqrt{1-\omega_0^2}}\right) \pm \epsilon_d\right], \quad (10)$$

where

$$\mathcal{D}(z) = z\left(\sqrt{1-z^2}+\Gamma\right) - \sqrt{\epsilon_d^2(1-z^2)+\Gamma^2\cos^2(\phi/2)}\,. \quad (11)$$

At the resonance ($\epsilon_d = 0$) in the limit $\Gamma \gg \Delta$, the expression is reduced to

$$\frac{A_{e(h)}}{\Delta} \approx 2\frac{\Delta^2}{\Gamma^2}\,. \quad (12)$$

Kondo correlated state behaves like a Fermi liquid. Naturally, if the reservoirs are normal metal, the Kondo resonance can be regarded in effect as a non-interacting resonance level at the Fermi energy E_F. In other words, many physical properties described pretty well by the effective impurity Green's function

$$G_d(z) = \frac{T_K/\Gamma}{z+iT_K} \quad (13)$$

with T_K playing the role of the level broadening. In the previous work[8] with particle-hole symmetry, it was demonstrated that this may also work for superconducting reservoirs. Indeed, the spectral weights in Fig. 4 fits very well to

$$\frac{A_{e(h)}}{\Delta} \sim \frac{\Delta^2}{T_K^2} \quad (14)$$

to be compared with Eq. (12).

True bound state Finally, we address whether the subgap Andreev state is a true bound state. Clerk et al. [33] and Sellier et al. [13] found finite broadening of the Andreev states. This may come from the finite temperature effects. The NCA cannot goes down to temperatures much lower than the Kondo temperature, and they worked at rather high temperatures[7, 13]. The spectrum from the NRG calculation is inherently discrete[34], and it is not easy to make a definite conclusion. However, as shown in Fig. 5, the subgap states are well separated from the continuum parts up to temperatures as high as the energy of the subgap states. At temperatures higher than the energy of the Andreev states, it is accompanied by other small spikes. It suggests that the subgap Andreev states are true bound states.

Conclusion We have studied the Kondo quantum dot coupled to two superconducting leads and investigated the subgap Andreev states using the NRG method. Contrary to the recent NCA results[7, 13], we observe Andreev states both below and above the Fermi level.

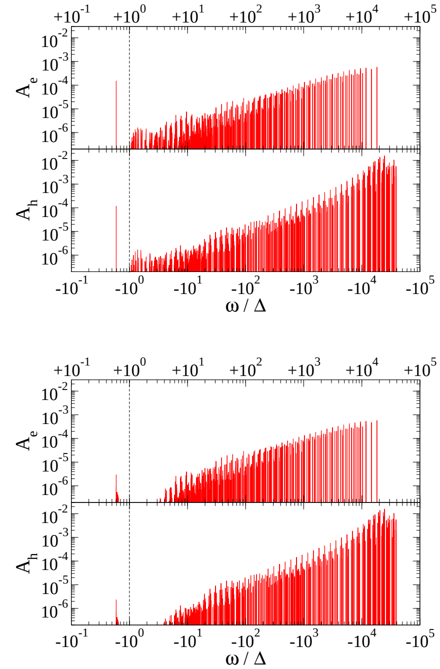

FIG. 5: (color on-line) Raw data of the spectral weights of the discrete energy levels from the NRG calculation (a) at $T = 0.1\Delta$ and (b) at $T = 0.5$.

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